

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 345 °C

Global applicability domain: Outside

Local applicability domain index: 2.67e-01

Confidence level: 4.77e-01

Nearest Neighbors from the Training Set

Image not found

Parathion

Measured: 375

Predicted: 362

Image not found

Benzene, 1,1'-sulfonylbis[4-methyl-

Measured: 406

Predicted: 360

Image not found

Diphenylsulfone

Measured: 279

Predicted: 315

Image not found

4,5-Dichlorophthalic anhydride

Measured: 313

Predicted: 312